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Reduced-dimensionality NMR spectroscopy for high-throughput protein resonance assignment.

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A suite of reduced-dimensionality (13)C,(15)N,(1)H-triple-resonance NMR experiments is presented for rapid and complete protein resonance assignment. Even when using short measurement times, these experiments allow one to retain the high spectral resolution required for efficient automated analysis. "Sampling limited" and "sensitivity limited" data collection regimes are defined, respectively, depending on whether the sampling of the indirect dimensions or the sensitivity of a multidimensional NMR experiments per se determines the minimally required measurement time. We show that reduced-dimensionality NMR spectroscopy is a powerful approach to avoid the "sampling limited regime"--i.e., a standard set of ten experiments proposed here allows one to effectively adapt minimal measurement times to sensitivity requirements. This is of particular interest in view of the greatly increased sensitivity of NMR spectrometers equipped with cryogenic probes. As a step toward fully automated analysis, the program AUTOASSIGN has been extended to provide sequential backbone and (13)C(beta) resonance assignments from these reduced-dimensionality NMR data.

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